Center Innovation Fund: ARC CIF

Computational Modeling of Ablative Materials: Application to Phenolic Pyrolysis

Completed Technology Project (2011 - 2012)

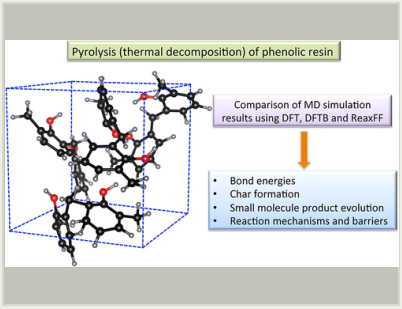
Project Introduction

Many NASA missions (ESMD, SMD), including crewed missions to Mars, are not possible with current ablative materials. Improved understanding will (1) facilitate the design of new, novel ablative materials and (2) improve material response models used for TSP design. We will demonstrate and validate phenolic pyrolysis simulation methods using reactive potentials (REAX), Density Functional Tight Binding (DFTB) and Density Functional Theory (DFT).

Ablative materials are required for the most demanding atmospheric reentry missions. These materials are often carbon fibers embedded in a phenolic polymer matrix. At high temperature, phenolic undergoes pyrolysis where the polymer is transformed into a pure carbon solid called char. Pyrolysis is an endothermic, chemically reactive process, and is the only in-depth energy absorbing mechanism used in ablative systems. High char yield is desirable to minimize mass loss into gaseous products. Importantly, polymer char yields can vary substantially. Further, thermal and mechanical properties of the pyrolyzed material can be very different from the original material. Optimizing properties of the char surface layer is crucial, since it is the part of the TSP in direct contact with the hot reentry plasma. A robust pyrolysis simulation methodology (which does not currently exist) will aid in understanding the structure and properties of phenolic and in developing new polymers with higher char yield and char with improved properties. In addition, more accurate material response models, used to design TSP, will result, thereby leading to reduced safety margins, and thus reduced mass/cost of the TPS. We will perform atomistic pyrolysis simulations using REAX, DFTB and DFT to demonstrate the different methods, and in particular to validate REAX for pyrolysis of realistic polymers (phenolic and otherwise). In addition, we will obtain important insights into chemical kinetics of early stage pyrolysis. These same methods can also be applied to other reactive processes (oxidation, sublimation, etc) and other problems in ablative materials modeling (polymer properties, interfaces, materials design, etc). This project resulted in the following journal publications: "Comparison of REAXFF, DFTB and DFT for Phenolic Pyrolysis. 1. Molecular Dynamics Simulations", T. Qi, C.W. Bauschlicher, J.W. Lawson, T.G. Desai, E.J. Reed, J. Phys. Chem. A 117, (2013), p. 11115 "Comparison of REAXFF, DFTB and DFT for Phenolic Pyrolysis. 2. Elementary Reaction Paths", C.W. Bauschlicher, T. Qi, E.J. Reed, A. Lenfant, J.W. Lawson, T.G. Desai, J. Phys. Chem. A 117, (2013), p. 11126

Anticipated Benefits

Many NASA missions (ESMD, SMD), including crewed missions to Mars, are not possible with current ablative materials. Computational modeling will enable the rapid and efficient development of the next generation of high performance ablators that are critical for NASA entry vehicles. We believe that this technology will enable ESMD and SMD missions.



Combination of molecular dynamics simulations and computational chemistry was used to study thermal decomposition of phenolic resins

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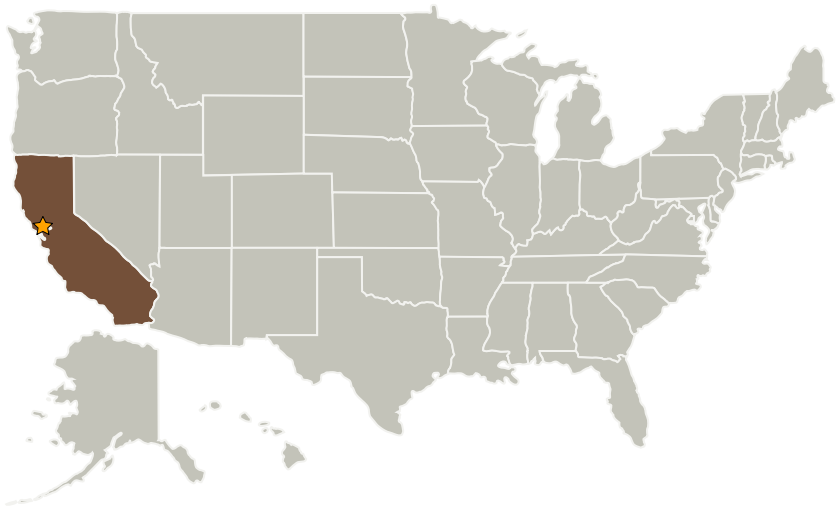
Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
★Ames Research Center(ARC)	Lead Organization	NASA Center	Moffett Field, California

Co-Funding Partners	Type	Location
Advanced Cooling Technologies, Inc.	Industry	Lancaster, Pennsylvania

Primary U.S. Work Locations
California

Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

Lead Center / Facility:

Ames Research Center (ARC)

Responsible Program:

Center Innovation Fund: ARC CIF

Project Management

Program Director:

Michael R Lapointe

Program Manager:

Harry Partridge

Project Manager:

John W Lawson

Principal Investigator:

John W Lawson

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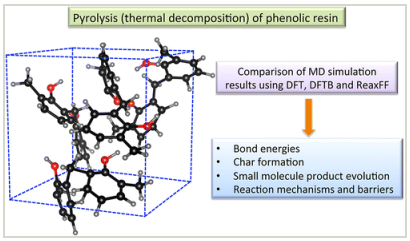
Images



Graphical abstract
Combination of molecular dynamics simulations and computational chemistry was used to study thermal decomposition of phenolic resins
(https://techport.nasa.gov/image/2963)

Stories

1676 Approval (# 17536)
(https://techport.nasa.gov/file/8728)

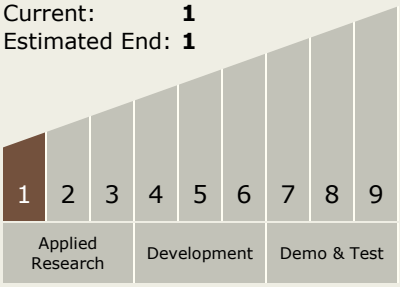
Links

Comparison of ReaxFF, DFTB, and DFT for Phenolic Pyrolysis. 1. Molecular Dynamics Simulations
(http://pubs.acs.org/doi/abs/10.1021/jp4081096)

Comparison of ReaxFF, DFTB, and DFT for Phenolic Pyrolysis. 2. Elementary Reaction Paths
(http://pubs.acs.org/doi/abs/10.1021/jp408113w)

Technology Maturity (TRL)

Start: **1**
Current: **1**
Estimated End: **1**



Technology Areas

Primary:

- TX14 Thermal Management Systems
  - TX14.3 Thermal Protection Components and Systems
    - TX14.3.1 Thermal Protection Materials